Quantum-and-Molecular Integrated Simulation of Thermal Properties of Nitrogen

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It is strongly desired to obtain thermal properties with enough accuracy through simulations. MD simulations seem to be one of the promising methods for this, but accuracy of the thermal properties obtained is often insufficient. We think this insufficiency mainly comes from accuracy of the intermolecular potential. In this study, to obtain thermal properties, we propose a new concept of simulations in which ab initio quantum simulation and molecular dynamics are integrated. We applied this concept to the calculation of thermal properties of nitrogen gas. At first, we calculated a 2-body intermolecular potential for N_2 using ab initio MO calculations and constructed a database. In the calculation, we examined effects of basis sets and electron correlation on the accuracy of the intermolecular potential. Next, we approximated this database by a function and considering the accuracy in this conversion. As we obtained the intermolecular potential of nitrogen, we conducted MD simulation to obtain thermal properties of N_2 gas and evaluated the intermolecular potential obtained and discussed possible improvements.